Wall-Enhanced Convection in Vibrofluidized Granular Systems

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An event-driven molecular dynamics simulation of inelastic hard spheres contained in a cylinder and subject to strong vibration reproduces accurately experimental results[1] for a system of vibrofluidized glass beads. In particular, we are able to obtain the velocity field and the density and temperature profiles observed experimentally. In addition, we show that the appearance of convection rolls is strongly influenced by the value of the sidewall-particle restitution coefficient. Suggestions for observing more complex convection patterns are proposed.

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INTRODUCTION

If sufficient power is supplied to a granular system contained in a cylindrical container by a vertically vibrating wall, fluidization occurs. Once a steady state is obtained, the energy input to the system by the wall is, on average, balanced by the energy dissipated in inelastic grain-grain and grain-wall collisions. This energy flux is responsible for various effects including non-linear temperature profiles, heap formation[2] and convection [1, 3]. Recent experiments using positron emission particle tracking (PEPT)[1] have observed buoyancy-driven convection in a highly fluidized granular system for a range of grain numbers and shaker amplitudes. While convection effects have been observed in a two-dimensional model system [4, 5], no simulation studies of a three dimensional system corresponding to the PEPT experiments have yet been reported.

We study the behavior of a model system in which the grains are modeled as inelastic hard spheres. Most of the previous studies of this model focused on the homogeneous cooling state, clustering, and kinetic and hydrodynamic theory for particles with small inelasticity[6, 7, 8]. Unlike many other many-body systems, the model studied here closely matches the experimental system. In particular, the number of particles is identical and we use values of particle-particle and particle-wall restitution coefficients that were determined by independent experimental measurements. We show that the model reproduces accurately the experimentally observed density and granular temperature profiles[9]. Moreover, for a range of conditions, a velocity field exists for which there is a net circulation. Interestingly, the direction and intensity of the circulation are strong functions of the particle-wall restitution coefficient. In addition, we suggest a modification to the experiment that may generate new convection patterns.

MODEL AND SIMULATION

The system consists of a number N of hard spheres contained in a cylinder of radius R. The spheres collide inelastically with each other and with the side walls with coefficients of restitution c and c_w, respectively. Between collisions, the spheres are subject to a downward constant acceleration due to the (vertical) gravitational field. Energy is injected into the system by the bottom wall which vibrates with a symmetric saw-tooth profile characterized by an amplitude A and a period T. We do not expect the behavior of the system to be strongly dependent on the form of the profile[10].

The equations describing the dynamics, which follow from conservation of momentum, for the particle sidewall, particle bottom-wall and particle particle collisions are:

$$\mathbf{v}'_{i,r} = \mathbf{v}_{i,r} - (1 + c_w)(\mathbf{v}_{i,r}.\hat{\mathbf{r}}_i)\hat{\mathbf{r}}_i \tag{1}$$

$$v'_{i,z} = 2v_w - v_{i,z} \tag{2}$$

$$\mathbf{v}'_{i,j} = \mathbf{v}_{i,j} \pm \frac{1+c}{2}[(\mathbf{v}_j - \mathbf{v}_i).\hat{\mathbf{n}}]\hat{\mathbf{n}} \tag{3}$$

respectively where $\mathbf{v}_{i,r}$ is the velocity of particle i in the x, y plane, v_w is the velocity of the bottom wall, $v_{i,z}$ is the z vertical component of the velocity of particle i, $\hat{\mathbf{r}}$ is the unit position vector of particle i and $\hat{\mathbf{n}}$ is the unit center-to-center vector between the colliding pair i and j. Note that we have taken the tangential restitution coefficient for sphere-sphere, and sphere-wall, collisions equal to one. The normal restitution coefficient for sphere-bottom wall collisions was also taken as unity.

One problem with the event-driven simulation is that a sphere may collide more and more frequently with the side wall as the radial component of its momentum is dissipated. To avoid the inelastic collapse[11], which has been observed in simulations of bulk granular systems,

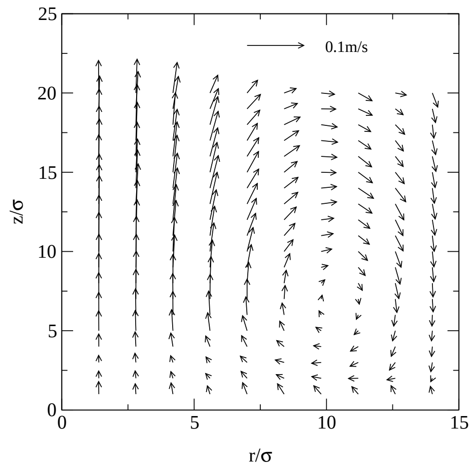

FIG. 1: Mean velocity field for a vibrofluidized system of inelastic hard spheres in the (r, z) plane. The wall-particle restitution coefficient is $c_w = 0.68$. Other parameters are given in the text

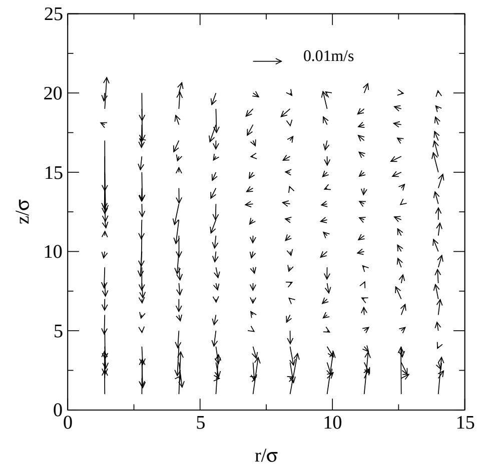

FIG. 2: Same as Figure 1 except that the wall-particle restitution coefficient is $c_w = 1.0$. Note that the velocities are much smaller than in Figure 1.

we simply inject a small amount of energy in the radial direction when the radial velocity falls below a cut-off value. This condition arises infrequently and its handling in this way has no discernible effect on the results.

To reproduce the experimental conditions of Wildman et al [1] we used parameter values $N = 1050$, $c = 0.91$, $c_w = 0.68$. Taking the unit of length as the sphere diameter, σ, the cylinder radius is $R/\sigma = 14$. Since the base-wall particle coefficient is not given, we assume a value of one. The shaker amplitude is thus left as the only adjustable parameter for the comparison of the simulation with the experiments. We performed different runs with a dimensionless shaking amplitude varying between 0.05 and 0.6. To generate the initial configuration, spheres were inserted sequentially and randomly in the cylinder without overlap. A preliminary simulation was then performed, typically for 5000 collisions per particle, in order to allow the system to reach the stationary non-equilibrium state.

Figure 1 displays the mean velocity field for the system of inelastic spheres in the (r, z) plane (r denotes the radial distance from the axis of the cylinder) when the reduced shaker amplitude is $A/\sigma = 0.32$. The field is averaged over the azimuthal angle and approximately 2×10^6 collisions). A torroidal convection roll is clearly present in which the particles flow, on average, up from the center and down the side wall. Note that, unlike the related Rayleigh-Bénard phenomenon, the roll is asymmetric. The velocity field is in near quantitative agreement with that observed experimentally by Wildman et al. [1]. In particular, the center of the vortex roll is at $(r/\sigma \simeq 10, z/\sigma \simeq 6)$ in reduced units which corresponds to $(r \simeq 50\text{mm}, z \simeq 30\text{mm})$ in experiments[1]. The shape of the roll, as well the location of its center, do not change appreciably as the shaker amplitude is varied between $0.28 \leq A/\sigma \leq 0.37$.

To highlight the role played by the wall, we performed additional simulations in which the wall-sphere collision is taken as elastic (a "perfect' wall for which the wall-particle restitution coefficient is equal to 1) with the other parameters unchanged. The mean velocity field of this simulation is quite different from the inelastic case. Although some convection is apparent in Figure 2, (particles on average flow up the wall and down to the center). It is weaker by about an order of magnitude in intensity (compare the velocity units at the top of Figs. 1 and. 2) and the roll direction is *opposite*.

To quantify the bulk convection, we have calculated the total velocity correlation, $C_{\text{tot}} = (1/N_c)\Sigma_{i,j}C(i,j)$[4] where (i,j) label the cells in the hydrodynamic region, N_c their total number and

$$C(i,j) = (1/8)\Sigma_{i',j'}\mathbf{v}(i,j).\mathbf{v}(i',j') \tag{4}$$

where the sum (i',j') is over the 8 neighboring cells of (i,j). See Figure 3. Bulk convection is present when C_{tot} is different from zero.

For $c_w = 0.68$, as the shaker amplitude is increased the total velocity correlation C_{tot} becomes different from zero when $A/\sigma > 0.05$, increases until $a/\sigma \simeq 0.2$ and stays roughly constant for larger amplitudes. A similar behavior was observed in the experiments of Wildman et al. [1]. For $c_w = 1$, C_{tot} is almost equal to zero for all amplitudes (Figure 3). A close examination of the corresponding flow velocity fields show that the amplitude of

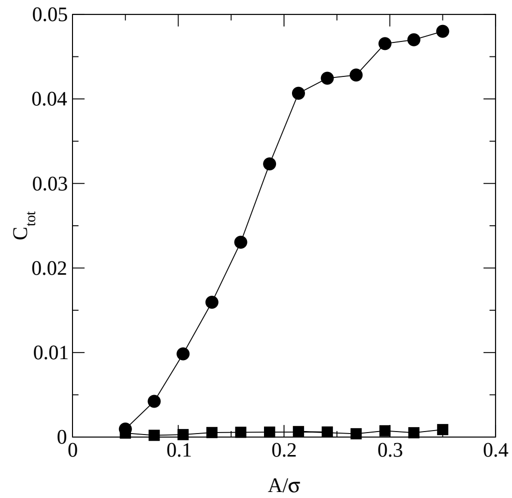

FIG. 3: Order parameter C_{tot} versus the shaker amplitude A/σ of the base wall. The squares and circles correspond to simulations where the wall-particle restitution coefficient is $c_w = 1.0$ and 0.68, respectively .

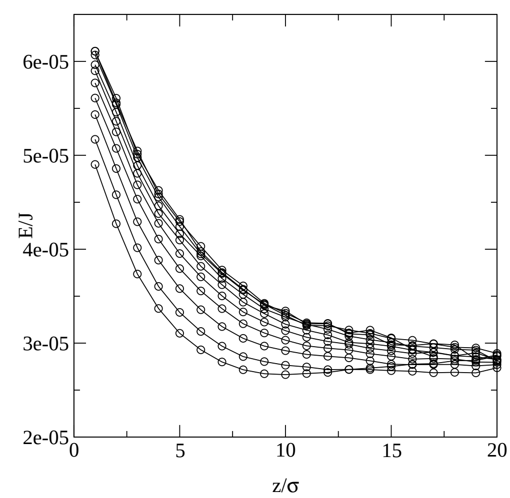

FIG. 4: Granular temperature for a vibrofluidized system of inelastic hard spheres as a function of the altitude z for different values of the radial position. From bottom to top, the curves correspond to $r/\sigma = 1.3, 2.6, 3.9, 5.2, 6.5, 7.8, 9.1, 10.4, 11.7, 13$. The particle mass is $1.875 \times 10^{-4} kg$.

the circulation of particles up the wall and down to the center exists for $A/\sigma > 0.05$, a feature which is not well handled by the calculation of the order parameter.

Figure 4 shows the granular temperature as a function of the altitude, z, for different values the radial position. These results agree well with the experiments (Fig.1 of Ref[1]) except for an underestimated maximum close to the basewall. These differences could result from the base-particle collisions which are assumed elastic in simulations. A minimum in the granular temperature profile is observed in the current simulations (and also in experiments) in the neighborhood of the center of the cylinder, but becomes weaker close to the wall cylinder. Fig 5 displays the same profiles for the system with $c_w = 1$: The temperature minimum in the vertical direction is more pronounced, but the temperature varies little in the radial direction. The existence of a minimum in the granular temperature along the z-direction is a phenomenon which is also present in the absence of convection[12] and results from the fact that at high altitudes the density and collision frequency are small, leading to a small number of hot particles.

Figure 6 displays a packing fraction plot which agrees qualitatively with the experimental results, except in the bottom region of the side wall where the density is higher than in experiments. Nevertheless, there is a maximum in the density profile in the vertical direction, whatever the radial distance. Moreover, there is also a maximum along the radial direction which is a consequence both of the compressible nature of the inelastic hard sphere system and of the small wall-particle restitution coefficient. When $c_w = 1$, the radial density gradient almost vanishes.

Although a complete theoretical treatment of the convection is beyond the scope of this Letter, we present some simple arguments that may help to rationalize the observed behavior. The Rayleigh-Bénard convection which is the paradigm for pattern formation in classical fluid mechanics, has been extensively studied over the past three decades[13, 14]. A temperature gradient applied to a fluid leads to a competition between buoyancy and disspation, which leads to the occurence of rolls above a threshold characterized by the non dimensional Rayleigh number R_a, which characterizes the ratio of the two forces. For larger temperature gradients, on observes a cascade of bifurcations ending in a chaotic regime.

For classical fluids, hydrodynamic equations reproduce the observed patterns remarkably well. The range of validity of continuum equations applied to granular materials, which contain a sink term in the energy equation to account for the dissipation of energy during collisions, is more restricted. Hydrodynamic equations can provide a good description of inelastic spheres [15], provided that the particles packing fraction remains $\eta > 0.04$ (below which the mean free path becomes comparable to the diameter of the cylinder). Similarly, if the packing fraction is too large ($\eta > 0.3$) the dissipation becomes too strong and the description breaks down. Using such an approach, Brey et al.[12] obtained temperature profiles

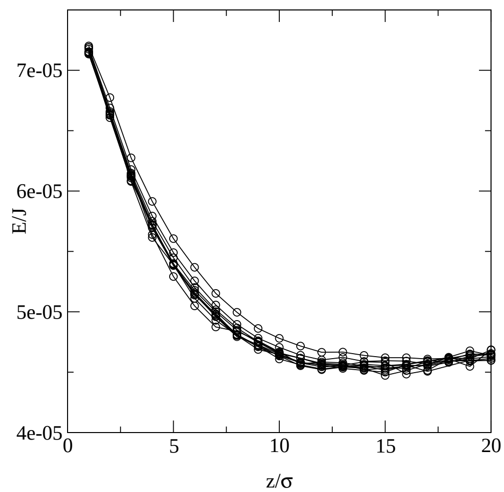

FIG. 5: Same as Figure 4 except $c_w = 1.0$. From top to bottom, the curves correspond to $r/\sigma = 13, 11.7, 10.4, 9.1, 7.86.5, 5.2, 3.9, 2.6, 1.3$.

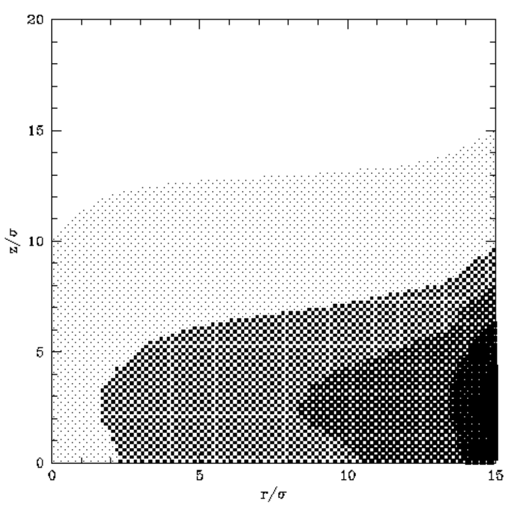

FIG. 6: Packing fraction (η) plot for the vibrofluidized system of inelastic hard spheres, with $c_w = 0.68$. The greyscale step corresponds to an η increase of 0.02 and white regions correspond to $\eta < 0.02$.

for an open granular system, *without convection* and predicted the presence of a minimum as a function of z, coinciding with the limit of validity of the hydrodynamic equations.

When $c_w = 0.68$, the hydrodynamic description breaks down close to the wall (high density and temperature gradient, strong dissipation). The onset of the bulk convective regime with a "real" wall is lowered because of the existence of the radial temperature gradient in addition to the vertical one. This can explain both the direction of circulation and the lowering of the threshold of convection compared to the case when the wall is perfect and no bulk convection is present. The circulation of particles is restricted close to the sidewall where strong dissipation is not well described by hydrodynamic equations. A kinetic approach is required close to the cylinder.

Our simulations clearly demonstrate the relevance of the inelastic hard sphere model for describing the experimental study of Wildman et al[1] and underline the key influence of the cylinder wall on the convection. Experimentally, unlike in the simulations, the wall-particle restitution coefficient is not an easily tunable parameter. We therefore propose a modification to the experiment that may lead to the observation of new phenomena. Specifically, we suggest adding an inner (solid) cylinder of a given radius, coaxial with the original cylinder. In the neighborhood of this inner cylinder, we expect particles to have a downward motion, and two, or more, toroidal rolls with alternate directions of circulation, as in a fluid system, might be produced.

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